

An Index Theorem for the Majorana Zero Modes in Chiral P-Wave Superconductors

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We show that the Majorana fermion zero modes in the cores of odd winding number vortices of a 2D $p_x + ip_y$ -paired superconductor is due to an index theorem. This theorem is analogous to that proven by Jackiw and Rebbi for the existence of localized Dirac fermion zero modes on the mass domain walls of a 1D Dirac theory. The important difference is that, in our case, the theorem is proven for a two component fermion theory where the first and second components are related by parity reversal and hermitian conjugation.

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The odd winding number vortices in a spinless (spin-polarized) $p_x + ip_y$ -paired superconductor or superfluid (for brevity we shall use “superconductor” to denote both in the rest of the paper) trap zero-energy bound states in the cores. The second-quantized operators creating these zero energy excitations are the self-hermitian, Majorana fermion operators. This property endows the vortices with non-Abelian statistics [1–3], which means that under braiding of any two vortices the total wavefunction transforms as a vector in a finite dimensional Hilbert space. Because of the non-Abelian statistics, this type of superconductor has been proposed to support topological quantum computation [2, 4, 5]. For example it has been shown that the Pfaffian $\nu = \frac{5}{2}$ fractional quantum Hall state [1, 6] is a spinless $p_x + ip_y$ superconductor of the “composite fermions” [1]. The braiding of non-Abelian quasiparticles in such a state [7] can, in principle, be exploited to build a quantum computer that is immune to environmental errors [8].

The root of the non-Abelian statistics is the presence of Majorana fermion zero modes in the vortex cores. Such zero modes were first proposed to exist in the vortex cores of the $p_x + ip_y$ -paired superfluid A-phase of Helium 3 in Ref. 9. Traditionally this peculiar kind of vortex core state was demonstrated by explicitly solving the Bogoliubov-de-Gennes (BdG) equations [1, 5, 10, 11]. Interestingly, the zero-energy solution is found only in the case when the winding number of the vortex is an odd integer (for even winding number vortices, there is no zero energy mode).

The zero mode in the vortex core discussed above is very analogous to the zero energy domain wall states of polyacetylene [14]. In that case, by writing down an ansatz for the dimerization-order-parameter profile, one can also demonstrate the existence of the zero energy domain wall solution by explicitly solving the mean-field equations [15]. Quite satisfactorily, this domain wall state was shown to be a condensed matter realization of the zero mode associated with the mass solitons of a 1D Dirac theory investigated earlier by Jackiw and Rebbi [12, 13].

The Jackiw and Rebbi soliton solution is a simple example of an index theorem where fermionic zero modes can be used to count the topological defects (or magnetic flux quanta) of a background order parameter (or magnetic field).

In this paper, we ask what the analogous index theorem is for the vortex Majorana fermion zero modes of a $p_x + ip_y$ superconductor. We proceed by mapping the 2D vortex problem on an effective 1D problem by performing angular momentum decomposition with respect to the center of the vortex. In this way, we can show that for odd winding number vortices there exists a *unique angular momentum channel* in which the following Hamiltonian describes the low energy quasiparticle excitations:

$$H_M = \int dx \left[-iv_F \chi^\dagger \sigma_z \partial_x \chi + m(x) \chi^\dagger \sigma_x \chi \right]. \quad (1)$$

In Eq. (1), $m(-x) = -m(x)$ is a spatially varying mass term that changes sign at $x = 0$ (the location of the domain wall), and $\chi^\dagger(x)$ is a two component field given by $\chi^\dagger(x) = (c^\dagger(x), c(-x))$, with $c(x)$ being a spinless fermion field. Note the important difference of Eq. (1) with the Dirac theory,

$$H_D = \int dx \left[-iv_F \psi^\dagger \sigma_z \partial_x \psi + m(x) \psi^\dagger \sigma_x \psi \right], \quad (2)$$

where $\psi^\dagger(x) = (f_1^\dagger(x), f_2^\dagger(x))$ with $f_{1,2}(x)$ being two *independent* fermion fields. It is because of such difference, the zero energy quasiparticles localized on the mass domain walls of Eq. (1) are Majorana fermions, while those localized on the domain walls of Eq. (2) are ordinary fermions. As we will show later, for even winding number vortices, such angular momentum channel does not exist.

We first briefly review the derivation of the Jackiw-Rebbi zero mode for Eq. (2). The quasiparticle operator

$$q^\dagger = \int dx [\phi_1(x) f_1^\dagger(x) + \phi_2(x) f_2^\dagger(x)]$$

satisfies $[H, q^\dagger] = \epsilon q^\dagger$. That implies the following Dirac equation for the two component wavefunction $\phi^T(x) = (\phi_1(x), \phi_2(x))$:

$$-iv_F \sigma_z \partial_x \phi(x) + \sigma_x m(x) \phi(x) = \epsilon \phi(x). \quad (3)$$

First we note that because σ_y anticommutes with σ_x and σ_z , if $\phi(x)$ is an eigenfunction with eigenvalue ϵ , $\sigma_y \phi(x)$ is also an eigenfunction with eigenvalue $-\epsilon$. As a result, the $\epsilon = 0$ solutions of Eq. (3) can be made a simultaneous eigenstate of σ_y . Let $\phi_0(x)$ denote such a solution and $\sigma_y \phi_0(x) = \lambda \phi_0(x)$. Set $\epsilon = 0$ and left-multiplying Eq. (3) by $i\sigma_z$ we obtain

$$\partial_x \phi_0(x) = \frac{\lambda}{v_F} m(x) \phi_0(x),$$

which implies

$$\phi_0(x) = e^{\frac{\lambda}{v_F} \int_0^x m(y) dy} \phi_0(0). \quad (4)$$

For $m(x) = \pm \text{sign}(x)|m(x)|$, Eq. (4) is normalizable for $\lambda = \mp 1$. In this way we have proven that for each sign change of $m(x)$ there is a single zero energy mode.

Now let us consider a uniform (i.e. with no vortices) 2D $p_x + ip_y$ superconductor. The fermionic mean-field Hamiltonian is given by $K + H_{0P}$, where

$$K = \sum_{\mathbf{k}} \xi_{\mathbf{k}} c_{\mathbf{k}}^\dagger c_{\mathbf{k}} \\ H_{0P} = -\Delta_0 \sum_{\mathbf{k}} (k_x + ik_y) c_{\mathbf{k}}^\dagger c_{-\mathbf{k}}^\dagger + \text{h.c.} \quad (5)$$

Here K is the kinetic energy term, H_{0P} is the pairing term and $\xi_{\mathbf{k}} = k^2/2m - \epsilon_F$ with ϵ_F the Fermi energy.

With the purpose of treating the electronic state of a single vortex in mind, we change to a new representation where the fermion operators are expanded in angular momentum channels,

$$c_{\mathbf{k}} = \frac{1}{\sqrt{2\pi k}} \sum_{m=-\infty}^{\infty} c_{m,k} e^{im\theta_{\mathbf{k}}},$$

with m an integer. The commutation relation $\{c_{\mathbf{k}}, c_{\mathbf{p}}^\dagger\} = \delta^2(\mathbf{k} - \mathbf{p})$ implies

$$\{c_{mk}, c_{np}^\dagger\} = \delta_{m,n} \delta(k - p).$$

Inserting them in Eq. (5), doing the $\theta_{\mathbf{k}}$ integral, and linearizing $\xi_{\mathbf{k}}$ around k_F , we get,

$$K = \frac{1}{(2\pi)^2} \sum_m \int_{-\Lambda}^{\Lambda} dq (v_F q) c_{m,q}^\dagger c_{m,q}, \quad (6)$$

where $q = k - k_F$, v_F is the Fermi velocity, and Λ is a momentum cut-off. So the kinetic energy term separates into uncoupled angular momentum channels indexed by

the integer angular momentum m . Using similar manipulations to decompose the pairing term, we find, using $\theta_{-\mathbf{k}} = \pi + \theta_{\mathbf{k}}$ and $k_x + ik_y = |k|e^{i\theta_{\mathbf{k}}}$,

$$H_{0P} = \frac{\Delta_0 k_F}{2\pi^2} \sum_m \int_{-\Lambda}^{\Lambda} dq \cos(m\pi) c_{m,q}^\dagger c_{1-m,q}^\dagger + \text{h.c.} \quad (7)$$

Putting Eq. (6) and Eq. (7) together we have, for each pair of m and $1 - m$, the following massive Dirac theory

$$H_m = \int dx \left[-iv_F' \psi_m^\dagger \sigma_z \partial_x \psi_m + m_0 \psi_m^\dagger \sigma_x \psi_m \right].$$

In the above, $\psi_m^\dagger(x)$ is the Fourier transform of $(c_{m,q}^\dagger, c_{1-m,q})$, $v_F' = \frac{v_F}{4\pi^2}$ and $m_0 = \frac{k_F \Delta_0 \cos(m\pi)}{2\pi^2}$. Consequently, all fermionic quasiparticle excitations are gapped.

Next we consider the fermionic Hamiltonian for a single winding number vortex located at the origin. The kinetic energy part of the Hamiltonian remains the same as in Eq. (6). Let us now consider the pairing term. In order to describe the spatial dependence of the superconducting order parameter, we start with the real space description,

$$H_{1P} = -\Delta_0 \int d^2 R \int d^2 r e^{i\theta_{\mathbf{R}}} h(R) g(\mathbf{r}) c_{\mathbf{R}+\mathbf{r}}^\dagger c_{\mathbf{R}-\mathbf{r}}^\dagger + \text{h.c.} \quad (8)$$

Here, \mathbf{R} and \mathbf{r} are the center-of-mass and the relative coordinates of the Cooper pair, respectively. $h(R)$ and $\theta_{\mathbf{R}}$ are the amplitude and the phase of the superconducting order parameter, and $g(\mathbf{r})$ is the Fourier transform of $(p_x + ip_y)$. In the vortex core, $h(R) \sim (1 - e^{-\frac{R}{\xi}})$ with ξ the coherence length. Substituting $c_{\mathbf{R}\pm\mathbf{r}}^\dagger = 2\pi \sum_{\mathbf{k}} c_{\mathbf{k}}^\dagger e^{i\mathbf{k}\cdot(\mathbf{R}\pm\mathbf{r})}$ in Eq. (8), we end up with two spatial integrals, $g(\mathbf{k} - \mathbf{p}) = \int d^2 r g(\mathbf{r}) e^{i(\mathbf{k}-\mathbf{p})\cdot\mathbf{r}} = (k_x - p_x) + i(k_y - p_y)$ and

$$I(\mathbf{k} + \mathbf{p}) = \int d^2 R e^{i\theta_{\mathbf{R}}} h(R) e^{i(\mathbf{k}+\mathbf{p})\cdot\mathbf{R}}. \quad (9)$$

In order to evaluate $I(\mathbf{k} + \mathbf{p})$, we first note that, $I(R_\theta(\mathbf{k} + \mathbf{p})) = e^{i\theta} I(\mathbf{k} + \mathbf{p})$, where R_θ is the operator that rotates $(\mathbf{k} + \mathbf{p})$ by an angle θ in the momentum space. It follows that, $I(\mathbf{k} + \mathbf{p}) = e^{i\theta_{\mathbf{k}+\mathbf{p}}} I(|\mathbf{k} + \mathbf{p}|)$. To evaluate $I(|\mathbf{k} + \mathbf{p}|)$ we choose $(\mathbf{k} + \mathbf{p})$ along the y -axis. Performing the $\theta_{\mathbf{R}}$ integral which produces $-2\pi i J_{-1}(|\mathbf{k} + \mathbf{p}|R)$, where J_{-1} is the Bessel function of the first kind of order -1 [16], and then performing the R integral which produces $\frac{(2\pi)^3 i}{|\mathbf{k} + \mathbf{p}|^2} \times \mathcal{O}(1)$, we find,

$$H_{1P} = -(2\pi)^3 i \Delta_0 \sum_{\mathbf{k}, \mathbf{p}} \frac{(k_x + ik_y)^2 - (p_x + ip_y)^2}{|\mathbf{k} + \mathbf{p}|^3} c_{\mathbf{k}}^\dagger c_{\mathbf{p}}^\dagger + \text{h.c.}$$

Finally, using angular momentum expansion of the fermion operators and noting that a function of $|\mathbf{k} + \mathbf{p}|$ is periodic in $(\theta_{\mathbf{k}} - \theta_{\mathbf{p}})$ and hence can be Fourier expanded

as

$$\frac{1}{|\mathbf{k} + \mathbf{p}|^3} = \sum_m u_m(k, p) e^{-im(\theta_{\mathbf{k}} - \theta_{\mathbf{p}})},$$

we rewrite H_{1P} as,

$$\begin{aligned} H_{1P} = & -(2\pi)^2 i \Delta_0 \sum_{\mathbf{k}, \mathbf{p}} \sum_{m, m_1, m_2} \left(\frac{k^2 e^{i2\theta_{\mathbf{k}}} p^2 e^{i2\theta_{\mathbf{p}}}}{\sqrt{kp}} \right) \\ & \times u_m(k, p) e^{-i(m_1+m)\theta_{\mathbf{k}}} e^{-i(m_2-m)\theta_{\mathbf{p}}} c_{m_1 k}^\dagger c_{m_2 p}^\dagger + \text{h.c.} \end{aligned} \quad (10)$$

Performing the $\theta_{\mathbf{k}}$ and $\theta_{\mathbf{p}}$ integrals in Eq. (10) for the two different terms, we get the conditions

$$m_1 = 2 - m, \quad m_2 = m, \quad \text{and} \quad m_1 = -m, \quad m_2 = 2 + m$$

respectively. Since $\frac{1}{|\mathbf{k} + \mathbf{p}|^3}$ depends on $\cos(\theta_{\mathbf{k}} - \theta_{\mathbf{p}})$, and hence is even in $(\theta_{\mathbf{k}} - \theta_{\mathbf{p}})$, $u_m(k, p) = u_{-m}(k, p)$. In addition, since $\frac{1}{|\mathbf{k} + \mathbf{p}|^3}$ is symmetric in the $\mathbf{k} \leftrightarrow \mathbf{p}$ exchange, $u_m(k, p) = u_m(p, k)$. Using these, we perform the transformation $m \rightarrow -m$ and interchange k and p in the second term of Eq. (10) to arrive at the simple form for the pairing term,

$$H_{1P} = -2i\Delta_0 \sum_m \int dk dp k^2 \sqrt{kp} u_m(k, p) c_{2-m, k}^\dagger c_{m, p}^\dagger + \text{h.c.} \quad (11)$$

In the above pairing Hamiltonian, each angular momentum channel m is coupled to channel $(2 - m)$. The only exception is the channel $m = 1$ which is decoupled from the rest. In this channel, writing $k = k_F + q$ and $p = k_F + q'$ for small q and q' , and noting that the coefficient of $c_{1, q}^\dagger c_{1, q'}$ must be odd in $(q - q')$ from the fermion anticommutation relation (otherwise, the integrals over q and q' in the pairing term below will give zero since the fermion bilinear changes sign under $q \leftrightarrow q'$), the Hamiltonian for the $m = 1$ channel takes the form,

$$\begin{aligned} H_1 = & \frac{1}{(2\pi)^2} \int_{-\Lambda}^{\Lambda} dq v_F q c_{1, q}^\dagger c_{1, q} + i\Delta_0 \int_{-\Lambda}^{\Lambda} dq dq' A(q - q') \\ & \times c_{1, q}^\dagger c_{1, q'}^\dagger + \text{h.c.} \end{aligned} \quad (12)$$

where $A(q - q')$ is an odd function of $(q - q')$, which, in leading order, is simply proportional to $(q - q')$. Defining a two component fermion operator $\chi_q^\dagger = (c_{1, q}^\dagger, c_{1, q})$, H_1 becomes Eq. (1) where $\chi^\dagger(x) = (c^\dagger(x), c(-x))$ is the Fourier transform of χ_q and $m(x)$ is the Fourier transform of $i\Delta_0 A(q)$. Due to the odd nature of $A(q)$, the mass term satisfies $m(-x) = -m(x)$.

Now we prove the index theorem for Eq. (1). By writing the quasiparticle operator as

$$\gamma^\dagger = \int dx [\eta_1(x) \chi_1^\dagger(x) + \eta_2(x) \chi_2^\dagger(x)]$$

where $\chi_1^\dagger(x) = c^\dagger(x)$ and $\chi_2^\dagger(x) = c(-x)$ and demanding that $[H, \gamma^\dagger] = \epsilon \gamma^\dagger$, we obtain the following equation for $\eta^T(x) = (\eta_1(x), \eta_2(x))$,

$$-iv_F \sigma_z \partial_x \eta(x) + m(x) \sigma_x \eta(x) = \frac{\epsilon}{2} \eta(x). \quad (13)$$

The rest of the proof for the zero mode is identical to that in the Dirac fermion case. To see that the zero energy quasiparticle is a Majorana fermion we recall that the zero energy solution of Eq. (13) is an eigenstate of σ_y . Explicitly it takes the form

$$\eta(x) = e^{\frac{\lambda}{v_F} \int_0^x m(y) dy} \frac{e^{i\pi/4}}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix}.$$

Here we have chosen a particular global phase for the σ_y eigenvector. Like the Dirac fermion zero modes, the value of λ here is ± 1 when the mass profile satisfies $m(x) = \mp \text{sign}(x) |m(x)|$. The corresponding quasiparticle operator takes the form,

$$\gamma^\dagger = \frac{1}{\mathcal{N}} \int dx e^{\frac{\lambda}{v_F} \int_0^x m(y) dy} \frac{e^{i\pi/4}}{\sqrt{2}} (c_1(x) - ic_1^\dagger(-x)), \quad (14)$$

where \mathcal{N} is a normalization factor. Since $e^{\frac{\lambda}{v_F} \int_0^x m(y) dy}$ is an even function of x (since $m(x)$ is an odd function), one can easily verify that $\gamma^\dagger = \gamma$, i.e., the quasiparticle is a Majorana fermion.

In angular momentum channels other than $m = 1$, channel m is coupled to channel $(2 - m)$. For these channels, the Hamiltonian is of the form

$$\begin{aligned} H_m = & \frac{1}{(2\pi)^2} \int_{-\Lambda}^{\Lambda} dq v_F q (c_{mq}^\dagger c_{mq} + c_{2-mq}^\dagger c_{2-mq}) \\ & + i\Delta_0 \int_{-\Lambda}^{\Lambda} dq dq' B(q, q') c_{mq}^\dagger c_{2-mq'}^\dagger + \text{h.c.} \end{aligned}$$

In this case there is no requirement that $B(q, q')$ has to change sign upon $q \leftrightarrow q'$ since the fermion operators in the pairing term are from two different angular momentum channels. Thus, generically, $B(0, 0)$ is non-zero, and the spectrum is gapped. In this case the real space Hamiltonian resembles Eq. (2) with $\psi^\dagger(x)$ the Fourier transform of $(c_{mq}, c_{2-mq}^\dagger)$, and the mass term does not change sign. Hence, there is exactly one zero mode in the spectrum.

For the system with a winding-number-two vortex, the factor $e^{i\theta_{\mathbf{R}}}$ in Eq. (8) is replaced by $e^{2i\theta_{\mathbf{R}}}$. This simple modification, as we show below, gets rid of the uncoupled angular momentum channel. Consequently, like the $m \neq 1$ angular momentum channels in the winding-number-one vortex discussed above, the real space Hamiltonian is of the form in Eq. (2) where the mass term does not change sign. Therefore the Jackiw-Rebbi theorem does not apply and there is no zero energy mode in the spectrum.

With the modification $e^{i\theta_{\mathbf{R}}} \rightarrow e^{2i\theta_{\mathbf{R}}}$ the function $I(\mathbf{k} + \mathbf{p})$ in Eq.(9) now satisfies, $I(R_{\theta}(\mathbf{k} + \mathbf{p})) = e^{2i\theta} I(\mathbf{k} + \mathbf{p})$. It follows that, $I(\mathbf{k} + \mathbf{p}) = e^{2i\theta_{\mathbf{k}+\mathbf{p}}} I(|\mathbf{k} + \mathbf{p}|)$. Doing similar calculation as earlier we obtain,

$$H_{2P} = -(2\pi)^2 \Delta_0 \sum_{\mathbf{k}, \mathbf{p}} \frac{r(k, p, \theta_{\mathbf{k}}, \theta_{\mathbf{p}})}{\sqrt{kp}} \sum_{m, m_1, m_2} v_m(k, p) \\ \times e^{-i(m_1+m)\theta_{\mathbf{k}}} e^{-i(m_2-m)\theta_{\mathbf{p}}} c_{m_1 \mathbf{k}}^{\dagger} c_{m_2 \mathbf{p}}^{\dagger} + h.c.,$$

where

$$r(k, p, \theta_{\mathbf{k}}, \theta_{\mathbf{p}}) = \left(k^3 e^{3i\theta_{\mathbf{k}}} + k^2 p e^{2i\theta_{\mathbf{k}}} e^{i\theta_{\mathbf{p}}} - p^2 k e^{2i\theta_{\mathbf{p}}} e^{i\theta_{\mathbf{k}}} \right. \\ \left. - p^3 e^{3i\theta_{\mathbf{p}}} \right).$$

and $v_m(k, p)$ is the Fourier component of $\frac{1}{|\mathbf{k} + \mathbf{p}|^4}$. Finally, performing the $\theta_{\mathbf{k}}$ and $\theta_{\mathbf{p}}$ integrals, and transforming $m \rightarrow -m$ along with interchanging k and p in the third and fourth terms of H_{2P} , we arrive at the equation analogous to Eq.(11),

$$H_{2P} = 2\Delta_0 \sum_m \int dk dp (k^3 + k^2 p) \sqrt{kp} v_m(k, p) \\ \times c_{3-m\mathbf{k}}^{\dagger} c_{mp}^{\dagger} + h.c.$$

It is clear from this equation that, in the case of the vortex with winding number two, no angular momentum channel in the pairing term decouples from the rest.

We can generalize the above calculations to the cases of arbitrary odd and even winding number vortices. For a vortex with an odd winding number, $2n - 1$, because of the factor $e^{i(2n-1)\theta_{\mathbf{R}}}$ in the pairing term, angular momentum channel m is coupled to channel $(2n - m)$. In this case, there is always a channel, $m = n$, which is decoupled from the rest. In this channel, quite generally, the Hamiltonian maps on Eq. (1) with a mass term which is an odd function simply because of the fermion anticommutation relation. The index theorem we proved in this paper then implies the existence of a zero energy Majorana fermion quasiparticle. In contrast, for a vortex with an even winding number, $2n$, angular momentum channel m is coupled to channel $(2n + 1 - m)$ by the pairing term. Consequently, like in the case of the vortex with winding number two, there is no decoupled angular momentum channel and there is no zero mode. Note that in the physics discussed above the breaking of time reversal symmetry is crucial, since, for 2D non-chiral p -wave superconductors, the bulk itself is gapless.

For s -wave superconductors, pairing occurs between the fermions with opposite spins. In this case, for a vortex with winding number one, one can show that the pairing term couples angular momenta m and $1 - m$, like in the uniform case discussed above. So there is no isolated channel. For a vortex with winding number two,

the channel $m = 1$ decouples, and the Hamiltonian in this channel takes the form

$$H_2 = \frac{1}{(2\pi)^2} \sum_{\sigma} \int_{-\Lambda}^{\Lambda} dq v_{Fq} c_{1q\sigma}^{\dagger} c_{1q\sigma} + \Delta_0 \int_{-\Lambda}^{\Lambda} dq dq' C(q, q') \\ \times c_{1q\uparrow}^{\dagger} c_{1,q'\downarrow}^{\dagger} + h.c.. \quad (15)$$

However, in Eq. 15, because of the opposite spins of the fermions in the pairing term, the anticommutation relations fail to produce an odd mass term. Thus, there is no zero mode at the vortices of an s -wave superconductor [17].

To conclude, we have proven an index theorem for the existence of zero modes in the vortex cores of chiral p -wave superconductors. The theorem, which is an analog of that in 1D Dirac fermion field theory with a mass soliton, correctly predicts a zero energy Majorana quasiparticle at the core of a vortex with odd winding number, and no such zero mode for a vortex with even winding number. The formalism also correctly captures the low energy quasiparticle physics at the vortex cores of s -wave superconductors.

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